A new extreme-scale parallel Poisson/Helmholtz solver combining local boundary integral equation and random walk methods

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I. Objective: We propose *a fundamentally new approach* of extreme-scale solvers for solving Poisson or reduced Helmholtz equations in complex 3-D geometries, with applications in many scientific and engineering problems including CFD, bio-electrostatics, and microchip design, etc.

The proposed approach is based on combining a deterministic (local) boundary integral equation and the random Brownian walk probabilistic Feynman-Kac representation of elliptic PDEs solutions. This hybridization allows us to produce a scalable parallel algorithm where the bulk of the computation has ***no need for cross-processor communication***, thus making the approach an ideal candidate for ***extreme-scale parallel and fault-resilient*** algorithm for up to millions of CPUs in the peta-flop/s computer systems.

The parallel algorithm to be developed will have the following salient features:

- *Non-iterative in construction and no need to solve any global linear system.*
- *Stochastic in nature based on Feynmann-Kac formula for elliptic PDEs.*
- *Massive parallelism suitable to large number of processors for exascale computing due to the random walk and local integral equation components of the algorithm.*
- *No need for traditional finite element type surface or volume meshes.*
- *Applicable to complex 3-D geometry with accurate treatment of domain boundaries.*
- *Resilience to random faults of processors in the multi-core computing architectures*.

II. Key idea: BIE-WOS, boundary integral equation (BIE) and walk on spheres (WOS) for computing DtN or NtD mapping for a general domain

The BIE-WOS method aims to find the DtN or NtD mapping of the PDE solution over boundary $\partial\Omega$ in a parallel manner by combining *local* integral equation and the random walk methods.

As shown in Fig.1, on a local patch $S \subset \partial\Omega$ we superimpose a "half" ball and the part of the ball outside the surface S is denoted by Ω_S with a boundary Γ. Let $G(x,y)$ be a Green's function of the ball which vanishes on its boundary (thus also on Γ being part of the sphere surface). Then, we have

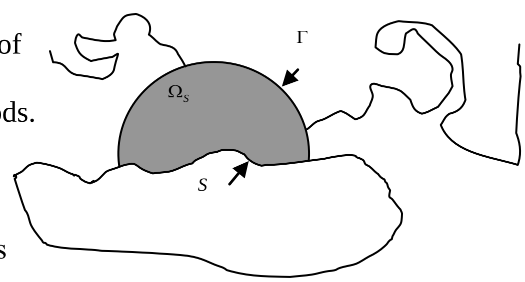

Fig. 1: BIE-WOS for local data on patch *S*

$$u(x) = \int_\Gamma \frac{\partial G}{\partial n} u(y) ds_y + \int_S [\frac{\partial G}{\partial n} u(y) + G \frac{\partial u}{\partial n}(y)] ds_y. \tag{1}$$

Next, by taking derivative of (1), we obtain the following hyper-singular boundary integral equation

$$\frac{1}{2}\frac{\partial u}{\partial n_x} = \int_\Gamma \frac{\partial^2 G}{\partial n_y \partial n_x} u(y) ds_y + p.f. \int_S [\frac{\partial^2 G}{\partial n_y \partial n_x} u(y) + \frac{\partial G}{\partial n_x}\frac{\partial u}{\partial n_y}] ds_y, \tag{2}$$

where the potential solution $u(y)$ is required on the hemisphere boundary Γ, and *both* Dirichlet and Neumann data on the boundary patch S are needed (one of them is given by PDE boundary conditions).

The **BIE-WOS** method consists of the following two steps:

Step 1: (WOS) random walks $X_t(\omega)$ based on walk on spheres (WOS) and the Feynman-Kac formula of Laplace solutions with a given Dirichlet data ϕ (Poisson equation can be treated similarly)

(3) $u(y) = E^y[\phi(X_{\tau_\Omega})]$, τ_Ω is the first hit time,

give the solution $u(y_{m,n})$ at 2-D Gauss points $y_{m,n} \in \Gamma$, allowing the integral over Γ by a quadrature

(4) $$\int_\Gamma \frac{\partial^2 G}{\partial n_y \partial n_x} u(y) ds_y \approx \sum_{m,n} \omega_{m,n} \frac{\partial^2 G(x, y_{m,n})}{\partial n_y \partial n_x} u(y_{m,n}), y_{m,n} \in \Gamma \cdot$$

Step 2: (BIE) with the integral over Γ found in (4), equation (2) implies that the Neumann data on the surface S will satisfy a second kind integral equation,

(5) $$(\frac{1}{2} I + K) \frac{\partial u}{\partial n}(x) = f(x), x \in S,$$

to be solved by a Nystr*ö*m collocation method for $x_n \in S$. Due to the small size of the selected patch S, the resulting small linear system can be inverted directly by Gauss elimination.

Alternatively, if the Neumann data is given on the boundary S, then the Dirichlet data $u(x)$ on S is desired, (1) can be used as a second kind of integral equation

(6) $$\left[\frac{1}{2} I + K\right] u(x) = h(x), x \in S.$$

Intrinsic Parallelism: the Neumann or Dirichlet data on each patch S on the boundary can be found from (5) or (6) without data exchanges from other patches, thus BIE-WOS can be scaled up for large number of CPUs. Once both the Neumann and Dirichlet data on the whole boundary are found, the solution in whole space can be obtained by the simple integral representation (done in one FMM implementation),

(7) $$u(x) = \int_{\partial\Omega} G(x,y) \frac{\partial u(y)}{\partial n_y} dy - \int_{\partial\Omega} \frac{\partial G(x,y)}{\partial n_y} u(y) dy$$

III. Preliminary Results:

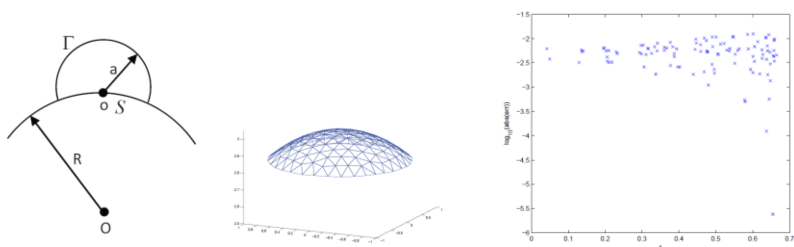

Fig 2 (left) a patch S for Neumann data, (middle) mesh on the patch, (right) error of BieWos

The BIE-WOS is used to find the Neumann data [1] on a patch S (Fig. 2(left)) where 10^4 Browian paths $X_t(\omega)$ are used in (3) for finding the solution $u(y_{m,n})$ on Γ for 30x30 Gauss points $y_{m,n}$ in (4), Fig 2 (right) shows the relative error for the Neumann data on the patch S at 10^{-2} with the BIE-WOS method.

IV. References:

[1] C.H. Yan, W. Cai, X. Zeng , A parallel method for solving Poisson equations with Dirichlet data using local boundary integral equations and random walks, submitted in revision to SIAM J. Scientific computing, , 1/2013. http://math2.uncc.edu/~wcai/BieWos.pdf